EXAMPLE

NSF Division of Chemistry Highlight Template

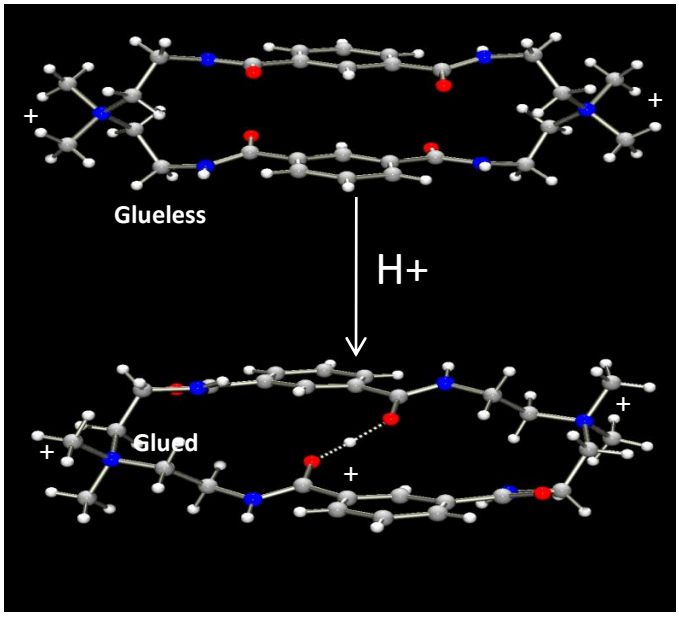
EXAMPLE

Principal Investigator Name/Institution: Kristin Bowman-James University of Kansas
Award Number: 0809736 (0316623)
Highlight Title: Hydrogen Bonds: Mother Nature's Glue

(choose an informative and engaging title, not the title of your grant)

Images: *Images are extremely important to publicize the results of NSF investments. In general, graphs, spectra, and reaction diagrams are not compelling to the general audiences for Highlights. Select images that best represent or capture the essence of the project outcome reported for this Highlight. Insert images in JPEG or GIF format, if possible. Provide a caption which clearly describes the image in lay terms with limited technical jargon . Provide a credit for all images.*

Image 1



Caption and Credit

Without any Hydrogen bonds (H-bonds), or "glueless," the top cyclic molecule is symmetrical. With a Low Barrier Hydrogen Bond (LBHB), or "glued," the bottom cyclic molecule is skewed. Unlike normal circumstances in which a positively charged atom or molecule is not attracted to another positively charged atom or molecule, the LBHB is unique in that it induces a positively charged molecule to be attracted to the positively charged hydrogen atom (H^+). Colors: red, oxygen; blue, nitrogen; gray, carbon; white hydrogen. Location of positive charges are indicated by $^+$.

Credit: Image provided by Kristin Bowman-James, Department of Chemistry, University of Kansas

Image 2

Caption 2 Professor Hossain (3rd from left) discovered the unusually strong Low Barrier Hydrogen Bond and is pictured with students at Jackson State University where he presently teaches chemistry and continues research on large molecule systems.

Credit 2 Picture provided by Kristin Bowman-James Department of Chemistry, University of Kansas

Project Outcome

The Bowman-James research group at the University of Kansas has discovered a Low Barrier Hydrogen Bond in a simple cyclic molecule. Low Barrier Hydrogen Bonds (LBHBs) occur when a hydrogen (H^+) atom links two atoms at very short distances. To date, LBHBs have only been suggested for proteins. However, if they are more prevalent than anticipated, as suggested by this finding, LBHBs could play major roles in protein folding, enzymatic activity, and ion channels. Unraveling the chemistry at the atomic level of this simple system may help explain more complex biological processes. Ultimately this knowledge may lead to more effective ways of addressing enzymatic "problems" such as diseases that affect living species. Hydrogen bonds (H-bonds) are weak interactions between a hydrogen atom and one other atom. H-bonds function as Nature's glue by influencing the shapes of molecules in catalysts, drugs, and biological macromolecules. H-bonds often help with the folding of enzymes, Nature's protein catalysts, into their catalytically active form. LBHBs are much stronger than H-bonds, however, they are less prevalent than normal H-bonds.

Use of X-ray crystallography to unravel the intricate workings of molecules has been an important goal of the Bowman-James group for over three decades. The technique was used to reveal the structure of the unusual phenomenon. A Post-doctoral Associate with Professor Bowman-James, Dr. Md. Alamgir Hossain, isolated and discovered the unusual cyclic molecule with the LBHB. He is currently an Assistant Professor at Jackson State University, where he mentors a number of underrepresented minority students and collaborates with Bowman-James.

*In the space above, provide a paragraph or two (about 300 words) that provides **results and outcomes of the project**, the scientific uniqueness; and the project's impact . Write the Highlight for a "lay audience"; lead-in sentence should engage the reader. Instead of starting with a lengthy explanation of the problem to be solved, start with a statement of what the research team has achieved, and only then go on to explain why it solves a problem or overcomes an obstacle and adds to scientific understanding.*

Does this Project Outcome Represent Potentially Transformative Research? If so, please provide explanation.

Yes

This simple and indeed serendipitous finding of an unusually strong Low Barrier Hydrogen Bond (LBHB) changing the shape of a cyclic molecule (macrocycle) illustrates the global importance of x-ray crystallography. Furthermore, the potentially transformative nature of the finding may indeed influence concepts about chemical bonding in biomacromolecular systems. The grant was also awarded a Creativity Extension.

Transformative Research Definition: Transformative research involves ideas, discoveries, or tools that radically change our understanding of an important existing scientific or engineering concept or educational practice or leads to the creation of a new paradigm or field of science, engineering, or education. Such research challenges current understanding or provides pathways to new frontiers. Transformative research results often do not fit within their established models or theories and may initially be unexpected or difficult to interpret; their transformative nature and utility might not be recognized until years later. Characteristics of transformative research are that it: challenges conventional wisdom, leads to unexpected insights that enable new techniques or methodologies, or redefines the boundaries of science, engineering, or education.

Please summarize the Intellectual Merit (technical significance and background) of this project outcome in a few sentences. Explain why this outcome is notable and/or important.

An unusually strong *LBHB* in a simple cyclic molecule (macrocycle) was discovered in Bowman-James' group using X-ray crystallography. Without H-bonds (glueless) the macrocycle is symmetrical. With the LBHB, the molecule skews and the oxygen-oxygen distance is a very short 2.45 Å, indicating a "single well potential" or equal pull by both oxygen atoms. What is amazing is that the macrocycle attracted another positively charged hydrogen ion when already carrying two plus charges, and that it formed such a strong LBHB! Comprehending the chemistry at the atomic level on a simple system will hopefully lead to a better understanding of the processes occurring in more complex biological systems and ultimately to more effective ways of addressing the enzymatic "problems," i.e., diseases, that affect living species.

Please summarize the major Broader Impacts of the project outcome in a few sentences. Explain why this outcome is notable and/or important. Broader Impacts include activities that advance discovery while teaching and training, seek to broaden participation of underrepresented groups, enhance infrastructure for research and education, disseminate information to enhance understanding of science and technology, and provide benefits to society.

The funded work in the Bowman-James group is disseminated by a variety of venues. During the project year 2007 Bowman-James was invited to present talks in Shanghai and Italy as well as in the United States. On these trips her postdoctoral associate, Dr. Sung Ok Kang, accompanied her, thus broadening Dr. Kang's experience in the scientific community. Bowman-James and Dr. Ben Hay (Oak Ridge National Laboratory) co-organized a symposium on Anion Coordination Chemistry at the National ACS meeting in Boston (Fall 2007). The entire Bowman-James research group attended the meeting and presented papers. The Postdoctoral Associate who led the discovery of the LBHB is now an Assistant Professor of Chemistry at a Historically Black University where he continues research on related topics and serves as a teacher, mentor, and advisor to a diverse group of students.

Publications Relevant to this Project Outcome

V. W. Da y, M. A. Hossain, S. O. Kang, D. Powell, G. Lushington, and K. Bowman-James, Encircled Proton, *J. Am. Chem. Soc.*, **2007**, *129*, 8692-9693 and *C & E News* **2007,** *85(27),* 24.

This project outcome was also featured in the FY2010 National Science Foundation Budget Request to Congress Mathematical & Physical Sciences Section

Provide a list of citations directly relevant to this outcome from publications in journals, newspapers, and various other media sources.

Website

http://www.chem.ku.edu/faculty/bowman/index.shtml

URL for project Website

Send the completed Highlight to the Division of Chemistry at:

chemhighlights@nsf.gov